CONTENTS

Polarized infrared spectra of $KHSO_4$ and $KDSO_4$ single crystals
J. Baran (Wrocław, Poland) 1
Solvent influence on rotational isomerism of chloroacetone
Z. Pawelka (Wrocław, Poland) 15
Hydrogen bonded complexes of methyl thiolacetate with proton donors: an infrared investigation in CCl_4 solution and in Ar matrices
A. Smolders, G. Maes and Th. Zeegers-Huyskens (Heverlee, Belgium) 23
The vibrational spectrum of $NaI \cdot 2X_2O$ (X = H or D)
I. Kanesaka and K. Kawai (Toyama, Japan) 41
IR spectra, methylene chain vibrations and rotational isomerism of n-alkyl trichloroacetates
Y. Mido, N. Komatsu (Kobe, Japan), J. Morcillo and M. V. Garcia (Madrid, Spain) 49
Spectral and structural study of the 4H-pyran ring containing an enaminoester moiety
J. Bellanato, F. Florencio, N. Martin and C. Seoane (Madrid, Spain) 63
Calculation of the vibrational spectra of cytosine derivatives by the CNDO/2 force method. Part I. Planar vibrations of 1-methylcytosine
K. Kuczera and M. Szczesniak (Warsaw, Poland) and K. Szczepaniak (Gainesville, FL, U.S.A.) 73
Calculation of the vibrational spectra of cytosine derivatives by the CNDO/2 force method. Part II. Planar vibrations of 5-fluorocytosine
K. Kuczera, M. Szczesniak (Warsaw, Poland) and K. Szczepaniak (Gainesville, FL, U.S.A.) 89
Calculation of the vibrational spectra of cytosine derivatives by the CNDO/2 force method. Part III. Planar vibrations of cytosine
K. Kuczera, M. Szczesniak (Warsaw, Poland) and K. Szczepaniak (Gainesville, FL, U.S.A.) 101
The vibrational spectra, structure, and conformational behavior of dimethyl dicarbonate
P. L. Lang and J. E. Katon (Oxford, OH, U.S.A.) 113
Infrared matrix isolation studies of the reactions of F_2 with sulfur and phosphorus bases
N. P. Machara and B. S. Ault (Cincinnati, OH, U.S.A.) 129
The ab initio analysis of molecular geometry and force fields in H_3XOXH_3 (X = C, Si) series
I. S. Ignatyev (Leningrad, U.S.S.R.) 139
Conformational behavior of 1-pentyne and 1-hexyne
G. A. Crowder (Canyon, TX, U.S.A.) 151
Formation of dimanganese heptoxide, Mn_2O_7, by photolysis of $Mn_2(CO)_{10}$ in O_2-doped argon matrices
M. J. Almond (Reading, Gt. Britain) 157
Vibrational assignment and conformational equilibrium for 3-fluoropropene based on ab initio calculations and high resolution far-infrared spectroscopy
J. R. Durig, T. J. Geyer, T. S. Little and D. T. Durig (Columbia, SC, U.S.A.) 165
Raman and far-infrared spectra of gaseous 1,1,1,3,3,3-hexafluoro-2-propanol, conformational stability and barriers to internal rotation
J. R. Durig, R. A. Larsen, F. O. Cox (Columbia, SC, U.S.A.) and B. J. van der Veken (Antwerp, Belgium) 183
Molecular structures of *trans* and *cis* 1,3-dibromo-1,3-dimethylcyclobutane studied by gas electron diffraction
T. Jonvik (Oslo, Norway), K. Griesbaum (Karlsruhe, F.R.G.) 203
Molecular structure and puckering potential of chlorocyclobutane studied by gas electron diffraction and Hartree–Fock calculations
T. Jonvik (Oslo, Norway) 213
Torsional potentials and conformational structures in chloro and bromo derivatives of propenal and propenoic acid obtained by molecular-mechanics calculations
G. O. Bostrøm, P. Bakken and R. Stølevik (Dragvoll, Norway) 227

Molecular structure and conformation of 2-acetyl-5-methyl-1,2,3-diazaphosphole: the use of ab initio calculations in an electron diffraction study
L. S. Khaikin, L. V. Vilkov (Moscow, U.S.S.R.) and J. E. Boggs (Austin, TX, U.S.A.) 241
The cumulant method in diffraction analysis of polyatomic molecules
A. A. Ischenko, V. P. Spiridonov, Yu. I. Tarasov and A. A. Stuchebryukhov (Moscow, U.S.S.R.) 255
Molecular structures of tert-butyl alcohol and tert-butyl methyl ether as studied by gas electron diffraction combined with vibrational spectroscopy
A. Suwa, H. Ohta and S. Konaka (Sapporo, Japan) 275
The conformations of 1,1,2,2-tetracyanoethane and 1,2-dichlorotetracyanoethane: a molecular orbital, dipole moment and Kerr effect study
Y. S. Chong, H. H. Huang (Kent Ridge, Singapore) and D. A. Winkler (Melbourne, Australia) 291
Normal coordinate analysis of CH_2ClSiX_3, $CHCl_2SiX_3$, CCl_3SiX_3 (X = H, D, F, Cl) molecules using Tikhonov's regularization method
I. V. Kochikov, G. M. Kuramshina, S. V. Syn'ko and Yu. A. Pentin (Moscow, U.S.S.R.) 299
The crystal and molecular structure of (−) *N*-[(*S*)-1-phenylethyl]-2-(*S*)-ethylsulfinyl-propenyl-1-amine
Z. Urbańczyk-Lipkowska, J. S. Krajewski, P. Gluziński, R. Kawęcki, L. Kozerski (Warsaw, Poland), G. D. Andreetti and G. Bocelli (Parma, Italy) 309
Electronic structure of metalloporphyrin π-anions
G. P. Gurinovich, I. F. Gurinovich, N. V. Ivashin, G. N. Sinyakov, A. M. Shulga, S. N. Terekhov, I. V. Filatov (Minsk, U.S.S.R.) and K. Dzilinski (Czestochowa, Poland) 317
202 MHz ^{31}P NMR performances. Part V. Two-dimensional ^{31}P NMR approaches in the cyclophosphazenic series
B. Perly, P. Berthault (Gif-sur-Yvette, France), L. Vidaud and J.-F. Labarre (Toulouse, France) 345
Unexpected chirality in *trans*-1,4-dicyanocyclohexane
M. Barón, J. A. Medrano, M. Ferraro and A. H. Buep (Buenos Aires, Argentina) 355
Solid-state structure and conformation of the cognition activator 3-phenoxypyridine sulphate: X-ray, two-dimensional ^1H NMR and ^{13}C NMR, and theoretical MO-MNDO studies
G. Bandoli (Padova, Italy), A. Grassi, E. Montoneri, G. C. Pappalardo (Catania, Italy) and B. Perly (Gif-sur-Yvette, France) 369
Synthesis and structural study of *N*-(8-isopropyl-northopan-3-α-yl)-2-methoxy-4-amino-5-chlorobenzamide
N. Cabezas, M. Martinez (Madrid, Spain), E. Galvez, M. S. Arias (Alcalá de Henares, Spain), F. Florencio and S. Garcia-Blanco (Madrid, Spain) 381
Conformational characterization of poly(L-phenylalanine) in the solid state by ^{13}C CP-MAS NMR spectroscopy
H. Miyamoto, R. Takezaki, T. Komoto, I. Ando, H. Saitô (Tokyo, Japan), T. Ozaki and A. Shoji (Gunma, Japan) 395
Crystallographic studies and physicochemical properties of π-electron compounds. Part XI. Crystal and molecular structure of sodium *p*-nitrobenzoate trihydrate
I. Turowska-Tyrk, T. M. Krygowski (Warsaw, Poland), M. Gdaniec (Poznań, Poland), G. Häfelinger and G. Ritter (Tübingen, F.R.G.) 401
Crystallographic studies and physicochemical properties of π-electron systems. Part XIV. Crystal and molecular structure of *N,N*-dimethyl-*p*-nitroanaline
J. Maurin and T. M. Krygowski (Warsaw, Poland) 413
The X-ray structure of 4-amino-7,8-dioxo-5,6,7,8-tetrahydro-1*H*-pyrazino[2,3-*c*]-1,2,6-thiadiazine-2,2-dioxide olate oxonium salt and the problem of the structure of the oxonium ion
J. Elguero, P. Goya, J. A. Paez, C. Foces-Foces, F. H. Cano and M. Martinez-Ripoll (Madrid, Spain) 423

Short Communication
Molecular mechanics calculations for some dimethylalkanes
G. A. Crowder (Canyon, TX, U.S.A.) 433

Book reviews 437

Corrigendum 441

Author Index 443

Subject Index 444